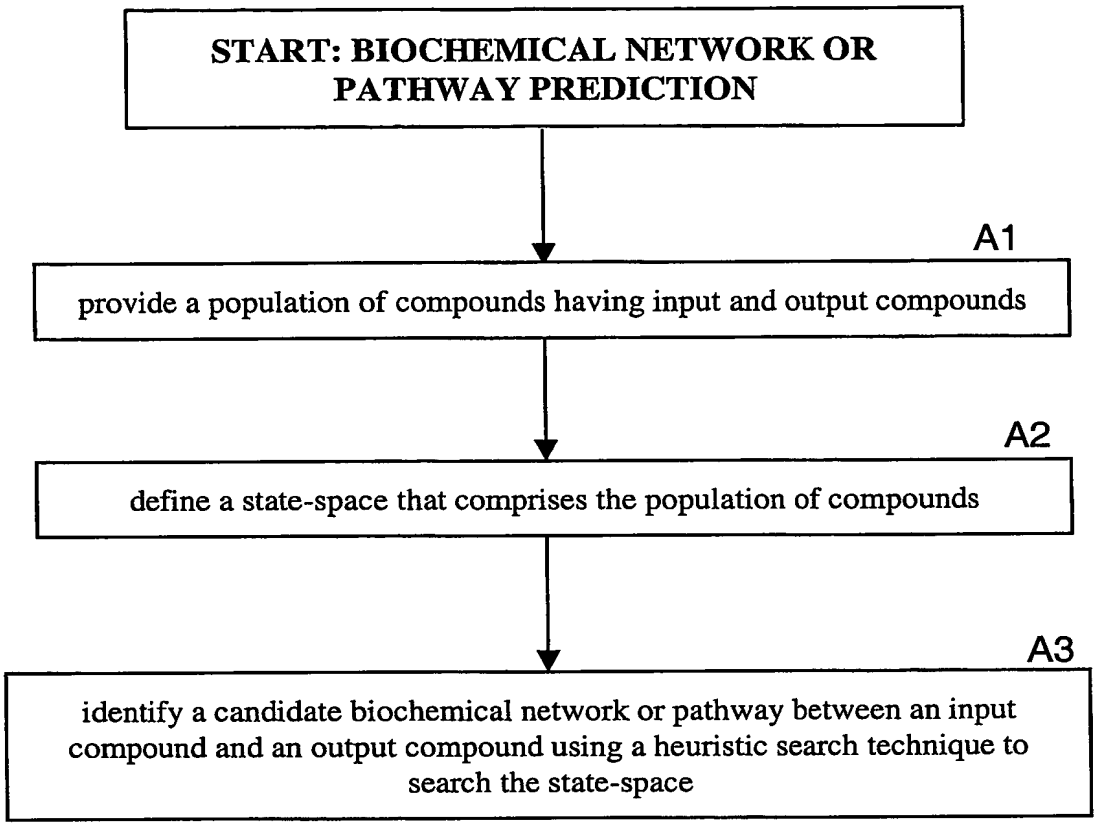

START: BIOCHEMICAL NETWORK OR PATHWAY PREDICTION
A1
provide a population of compounds having input and output compounds
A2
define a state-space that comprises the population of compounds
A3
identify a candidate biochemical network or pathway between an input compound and an output compound using a heuristic search technique to search the state-space

Fig. 1

```
(AG AS AU BI BR C CA CD CL CO CU F FE GA H H+ HG I K LI MG MN MO N NA
 NI O P PB PT R S SB SE SI SN TC TE W X ZN BR-R C#C C#N C#O C-*
 C-AS C-BR C-C C-CL C-CO C-F C-FE C-H C-HG C-I C-MO C-N C-O C-P C-R C-S
 C-SE C-SI C-SN C-TC C-TE C-X C=C C=N C=O C=R C=S CL-CA CL-FE CL-HG
 CL-MG CL-PT CL-R H-CL H-N H-O HG-R I-I I-R K-I N#N N-* N-CO N-FE
 N-MG N-N N-NI N-O N-P N-PT N-R N-S N-SN N-X N-ZN N=N N=O N=P N=S O-*
 O-AS O-BI O-CA O-CL O-CO O-FE O-HG O-K O-MG O-NA O-O O-P O-R O-S O-SB
 O-SE O-SI O-SN O=AS O=CL O=O O=P O=S O=SE P-F P-S P=AU P=S P=SE S-AS
 S-AU S-F S-FE S-HG S-MO S-R S-S SE-SE)
```

Fig. 2

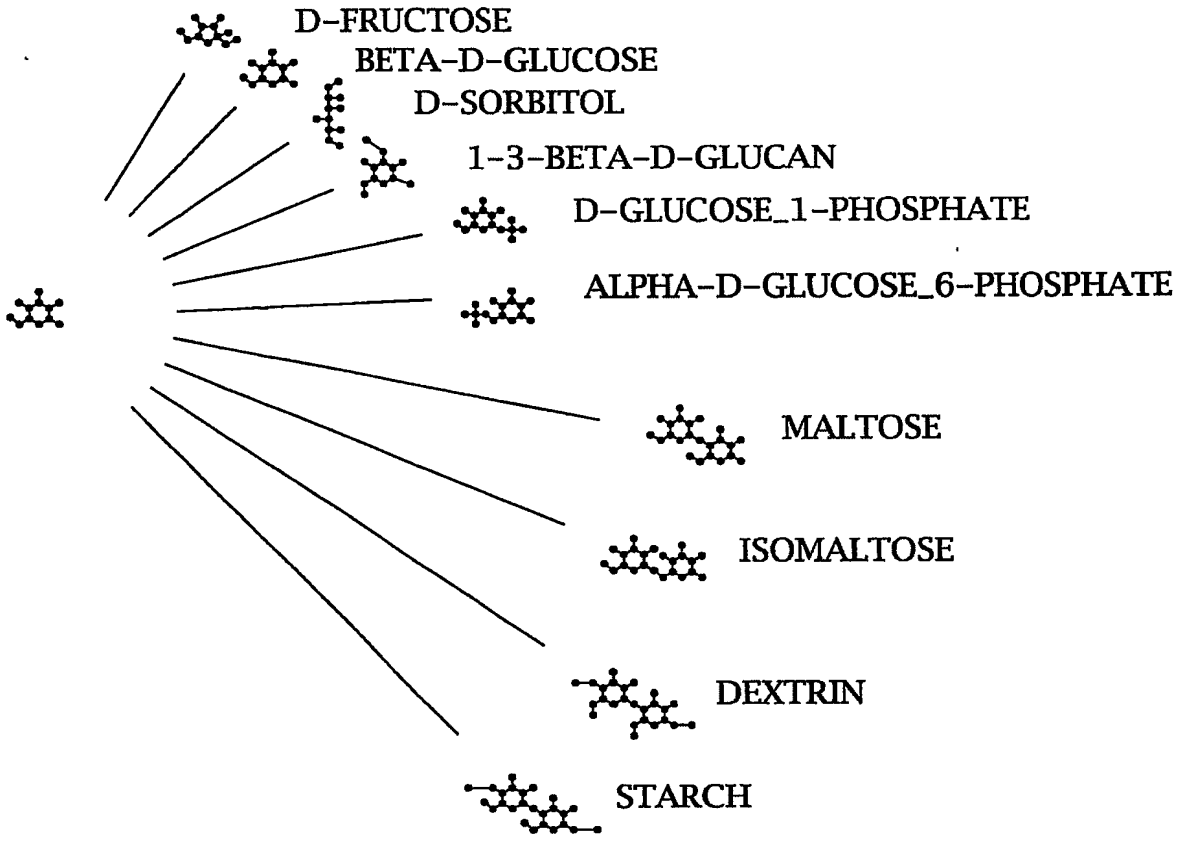

D-FRUCTOSE
BETA-D-GLUCOSE
D-SORBITOL
1-3-BETA-D-GLUCAN
D-GLUCOSE_1-PHOSPHATE
ALPHA-D-GLUCOSE_6-PHOSPHATE
MALTOSE
ISOMALTOSE
DEXTRIN
STARCH

Fig. 3

```
input  : x^0, x^L, F
output : P^{0,L}
begin
    X ← (x^0), P^{0,L} ← ()
    while X ≠ () do
        x ← argmax(F(x^i); x^i ∈ X)
        T ← successors(x)
        for x^m ∈ T do
            if x^m = x^L then
                P^{0,L} ← path(x^m)
                return P^{0,L}
            if x^m ∉ X then
                push (x^m, X)
                point(x^m, x)
            else
                if F(x^m) < F(x^m)|_old then
                    point(x^m, x)
end
```

Fig. 4

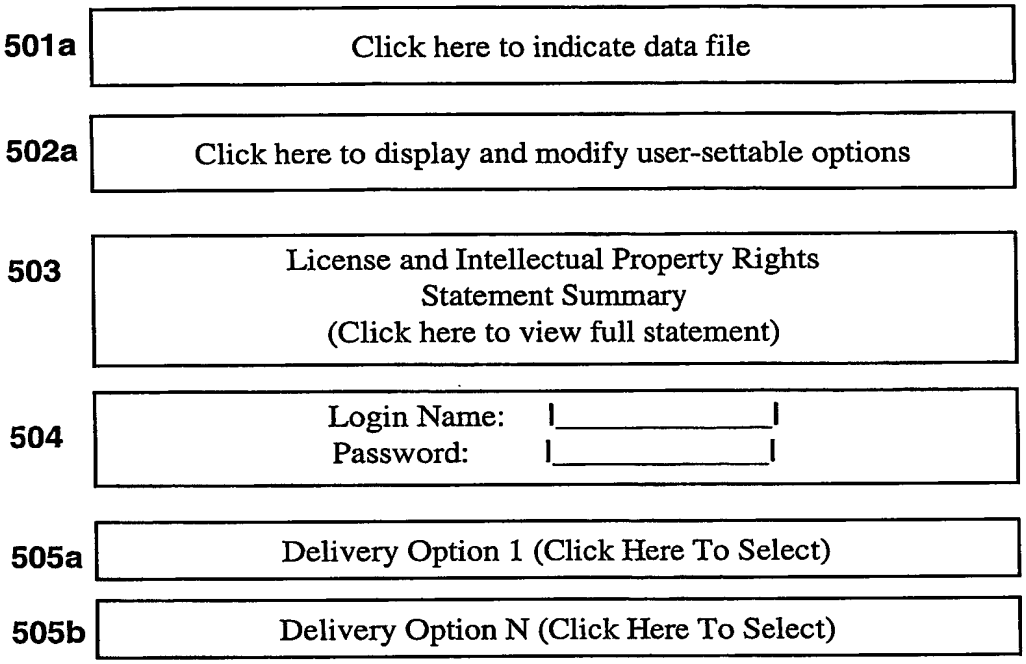

501a
Click here to indicate data file
502a
Click here to display and modify user-settable options
503
License and Intellectual Property Rights
Statement Summary
(Click here to view full statement)
504
Login Name: |_____|
Password: |_____|
505a
Delivery Option 1 (Click Here To Select)
505b
Delivery Option N (Click Here To Select)

Fig. 5A

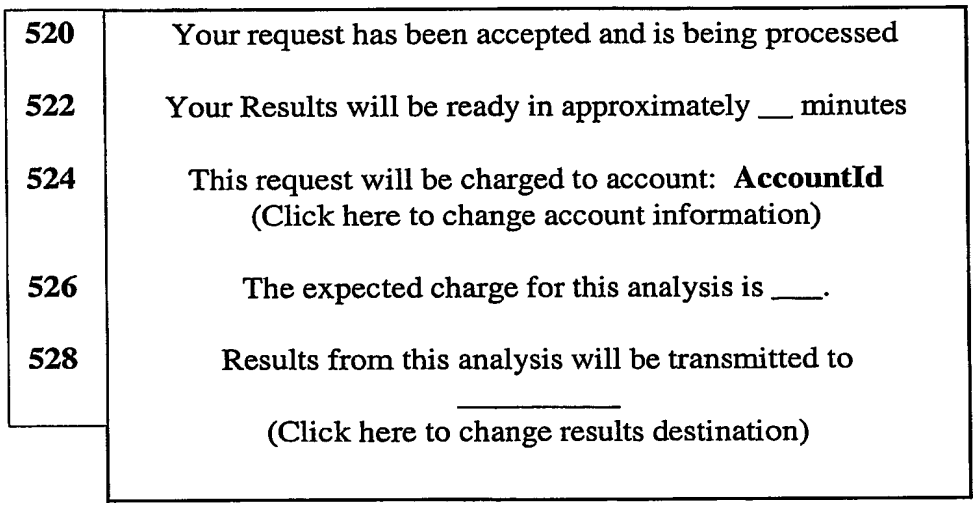

520
Your request has been accepted and is being processed
522
Your Results will be ready in approximately __ minutes
524
This request will be charged to account: **AccountId**
(Click here to change account information)
526
The expected charge for this analysis is ___.
528
Results from this analysis will be transmitted to
_____
(Click here to change results destination)

Fig. 5B

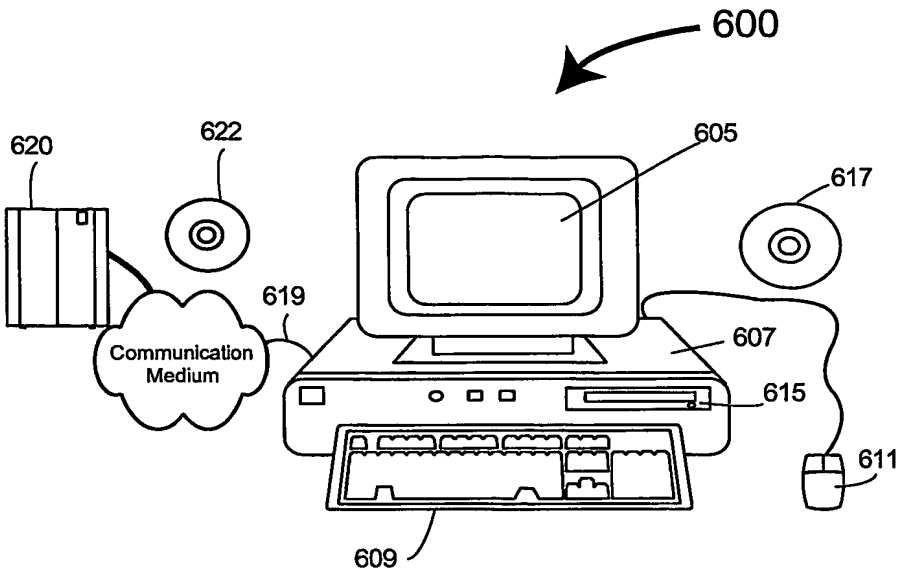

600
620
622
605
617
619
Communication Medium
607
615
611
609

Fig. 6

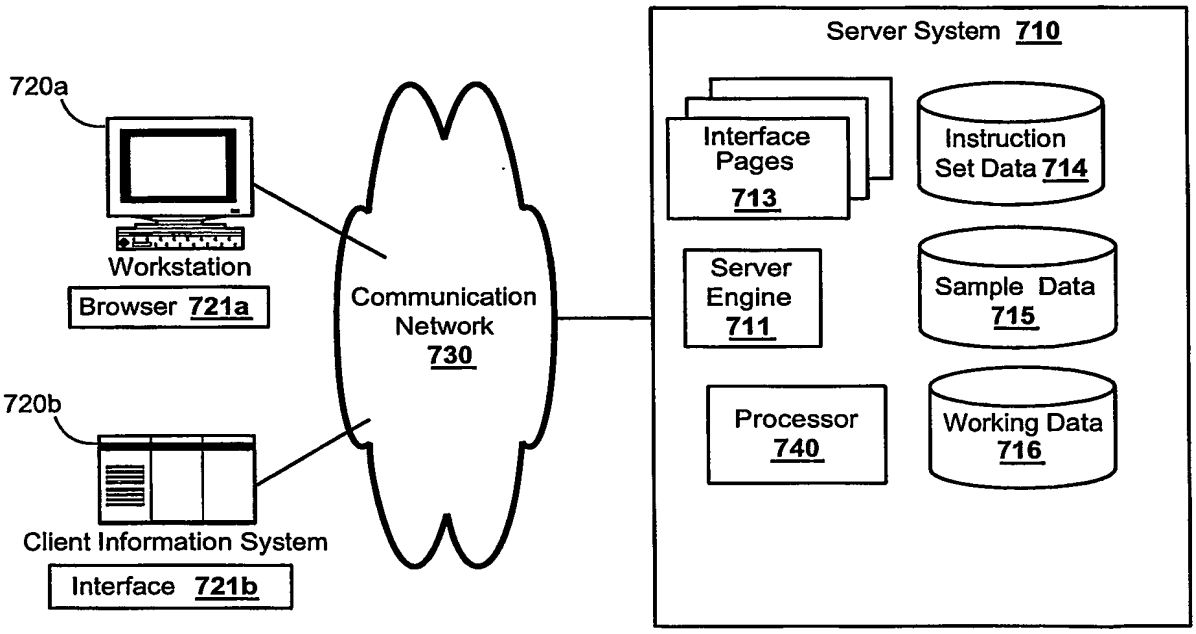

Server System 710
720a
Workstation
Browser 721a
Communication Network 730
Interface Pages 713
Instruction Set Data 714
Server Engine 711
Sample Data 715
Processor 740
Working Data 716
720b
Client Information System
Interface 721b

Fig. 7

Example (a)
From: α-D-Glucose
To : pyruvate

Alg	M	L	F	b*	t(s)
BFS	209	5	29	2.65	8.86
DFS	26	22	491	1.01	1.64
A*	27	6	29	1.44	1.83

Example (b)
From: citrate
To : L-tyrosine

Alg	M	L	F	b*	t(s)
BFS	126	3	37	4.63	6.76
DFS	4718	123	2013	2.00	69.14
A*	20	6	13	1.34	1.98

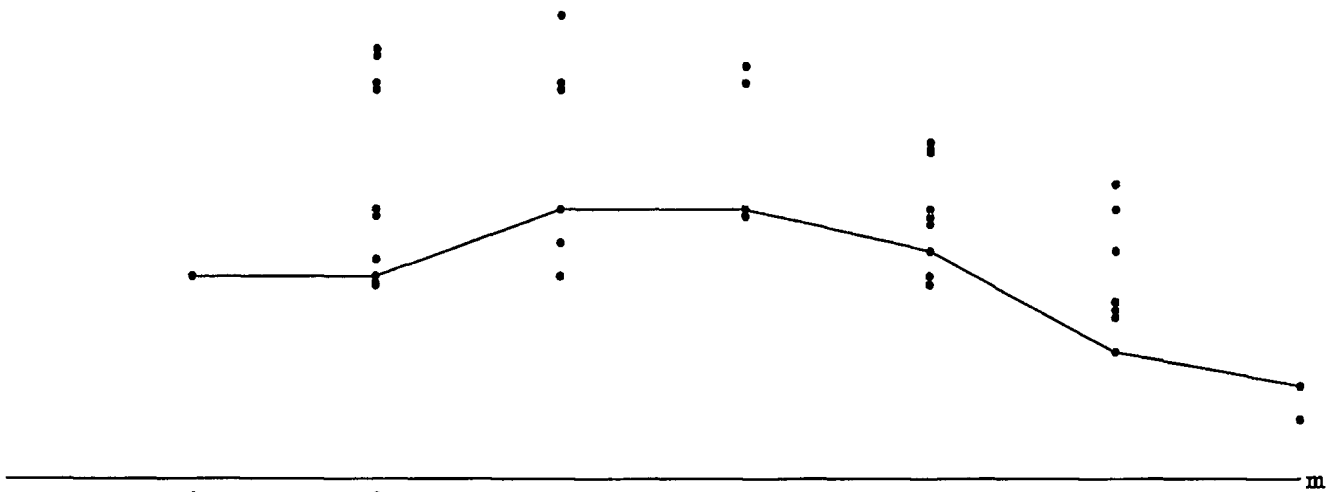
Example (c)
From: α-D-glucose
To : 1,3-propanediol

Alg	M	L	F	b*	t(s)
BFS	652	7	81	2.33	19.42
DFS	19	17	185	1.01	1.83
A*	112	7	31	1.74	6.90

Example (d)
From: citrate
To : L-histidine

Alg	M	L	F	b*	t(s)
BFS	653	6	45	2.73	16.97
DFS	-	-	-	-	$> 10^4$
A*	72	7	15	1.61	4.20

Fig. 8



m	0	1	2	3	4	5	6
Features	24	24	32	32	27	15	11
Successors	10	7	5	11	8	3	46
G(0,m)	0	0	8	8	13	25	29
H(m,L)	13	13	21	21	16	4	0
F(0,m,L)	13	13	29	29	29	29	29
EC		5.1.3.3	2.7.1.63	5.3.1.9	2.2.1.1	4.1.2.9	1.2.3.3

0 ALPHA-D-GLUCOSE	((C 6) (O 6) (C-C 5) (C-O 7))	
1 BETA-D-GLUCOSE	((C 6) (O 6) (C-C 5) (C-O 7))	ALDOSE_1-EPIMERASE
2 BETA-D-GLUCOSE_6-PHOSPHATE	((C 6) (O 9) (P 1) (C-C 5) (C-O 7) (O-P 3) (O=P 1))	POLYPHOSPHATE-GLUCOSE_PHOSPHOTRANSFERASE
3 BETA-D-FRUCTOSE_6-PHOSPHATE	((C 6) (O 9) (P 1) (C-C 5) (C-O 7) (O-P 3) (O=P 1))	GLUCOSE-6-PHOSPHATE_ISOMERASE
4 D-XYLULOSE_5-PHOSPHATE	((C 5) (O 8) (P 1) (C-C 4) (C-O 4) (C=O 1) (O-P 3) (O=P 1))	TRANSKETOLASE
5 ACETYL_PHOSPHATE	((C 2) (O 5) (P 1) (C-C 1) (C-O 1) (C=O 1) (O-P 3) (O=P 1))	PHOSPHOKETOLASE
6 PYRUVATE	((C 3) (O 3) (C-C 2) (C-O 1) (C=O 2))	PYRUVATE_OXIDASE

Fig. 9

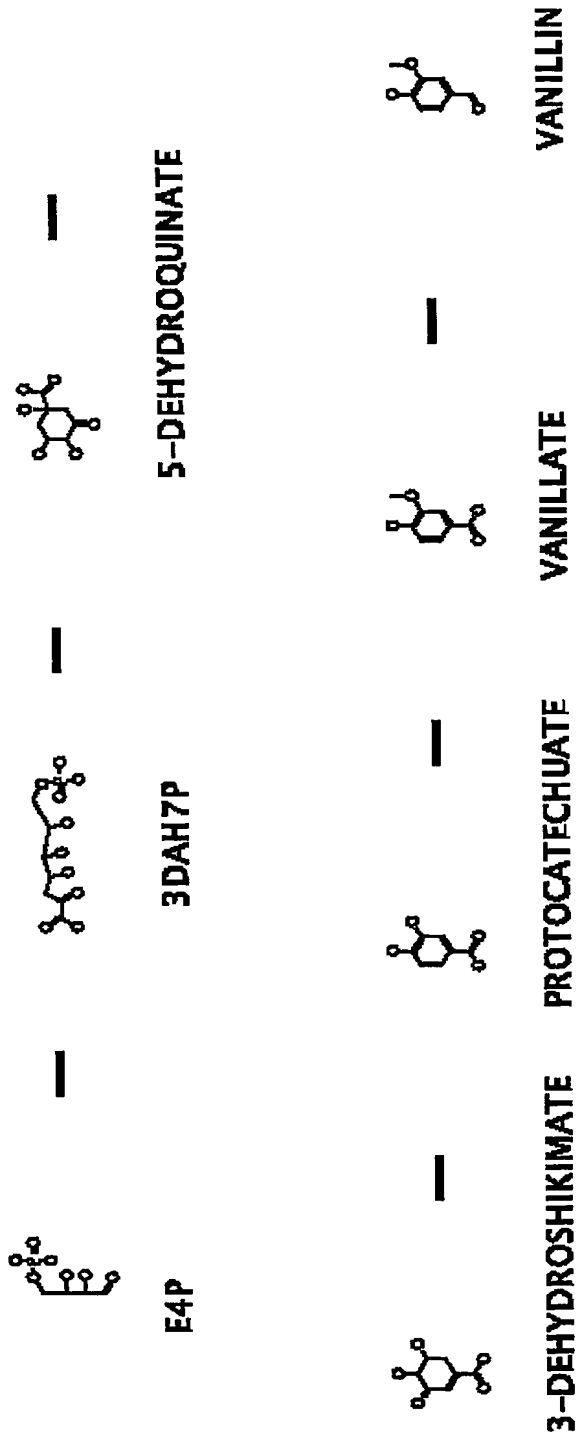
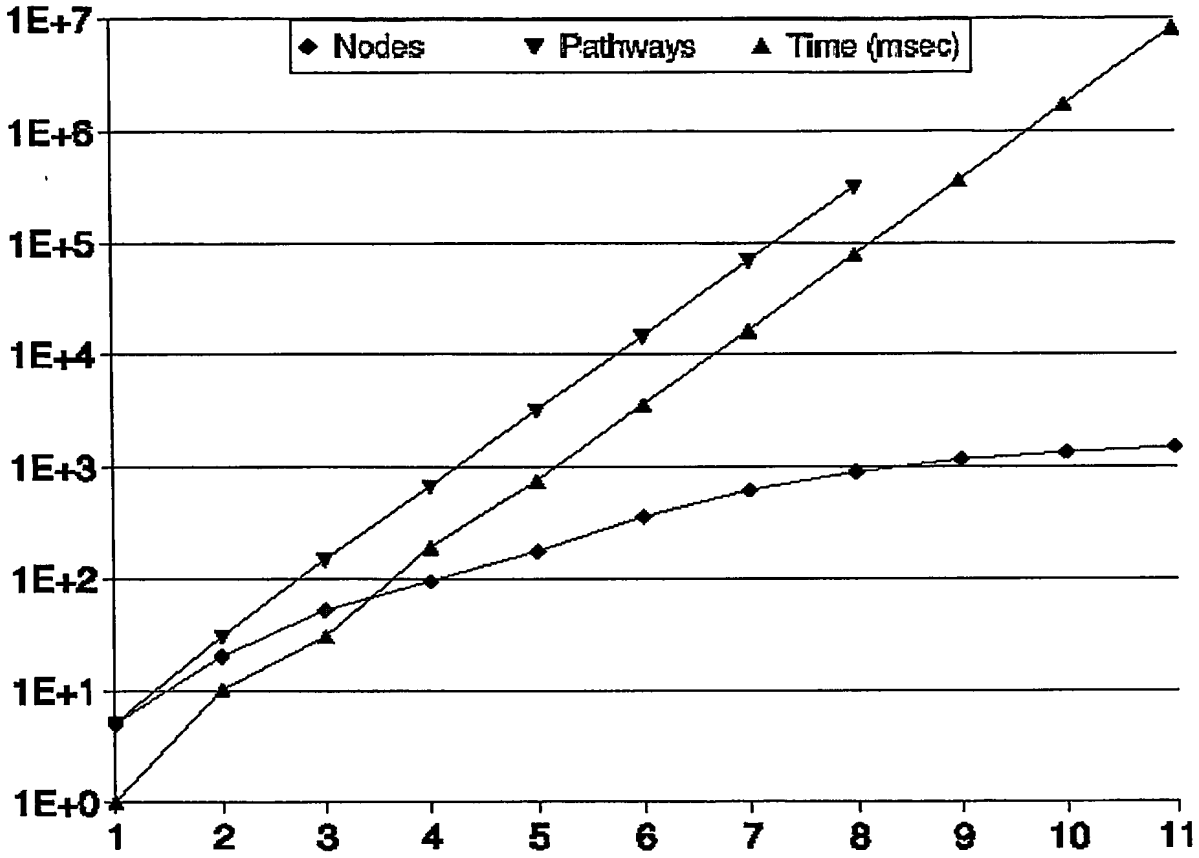

E4P
3DAH7P
5-DEHYDROQUINATE
3-DEHYDROSHIKIMATE
PROTOCATECHUATE
VANILLATE
VANILLIN

Fig. 10

```
input : x^0, x^L, Ω
output: P^{0,L}
begin
    N← make-node(x^0)
    while N≠ () do
        n ← pop(N)
        P^{0,L} ← node-solution(n)
        if goal-test(n) then
            return P^{0,L}
        for (reaction,compound) ∈ successors(n) do
            e ← edge-cost(n reaction compound)
            h ← h-cost(compound)
            g ← g-cost(n) + e
            f ← g + h
            d ← depth(n)
            n' ← make-node(n reaction compound g h f d)
            push(n' N)
        N ← sort(N f-cost)
end
```

Fig. 11



Variable	Regression
Nodes	$= 7.87 \times 1.73^{x}$
Paths	$= 1.23 \times 4.77^{x}$
Time	$= 0.31 \times 4.74^{x}$

Fig. 12

ALPHA-D-GLUCOSE + 2 ATP + 2R-2-HYDROXY-3-PHOSPHONOOXY-PROPANAL + PHOSPHOENOLPYRUVATE + NADH + OXYGEN + PYRUVATE + S-ADENOSYL-L-METHIONINE + COA => ADP +D-XYLULOSE_5-PHOSPHATE + 2 ORTHOPHOSPHATE + 3 H2O + CO2 + NAD+ + S-ADENOSYL-L-HOMOCYSTEINE + PRODUCTS_OF_ATP_BREAKDOWN + 4-HYDROXY-3-METHOXY-BENZALDEHYDE +ACETYL-COA

Fig. 13

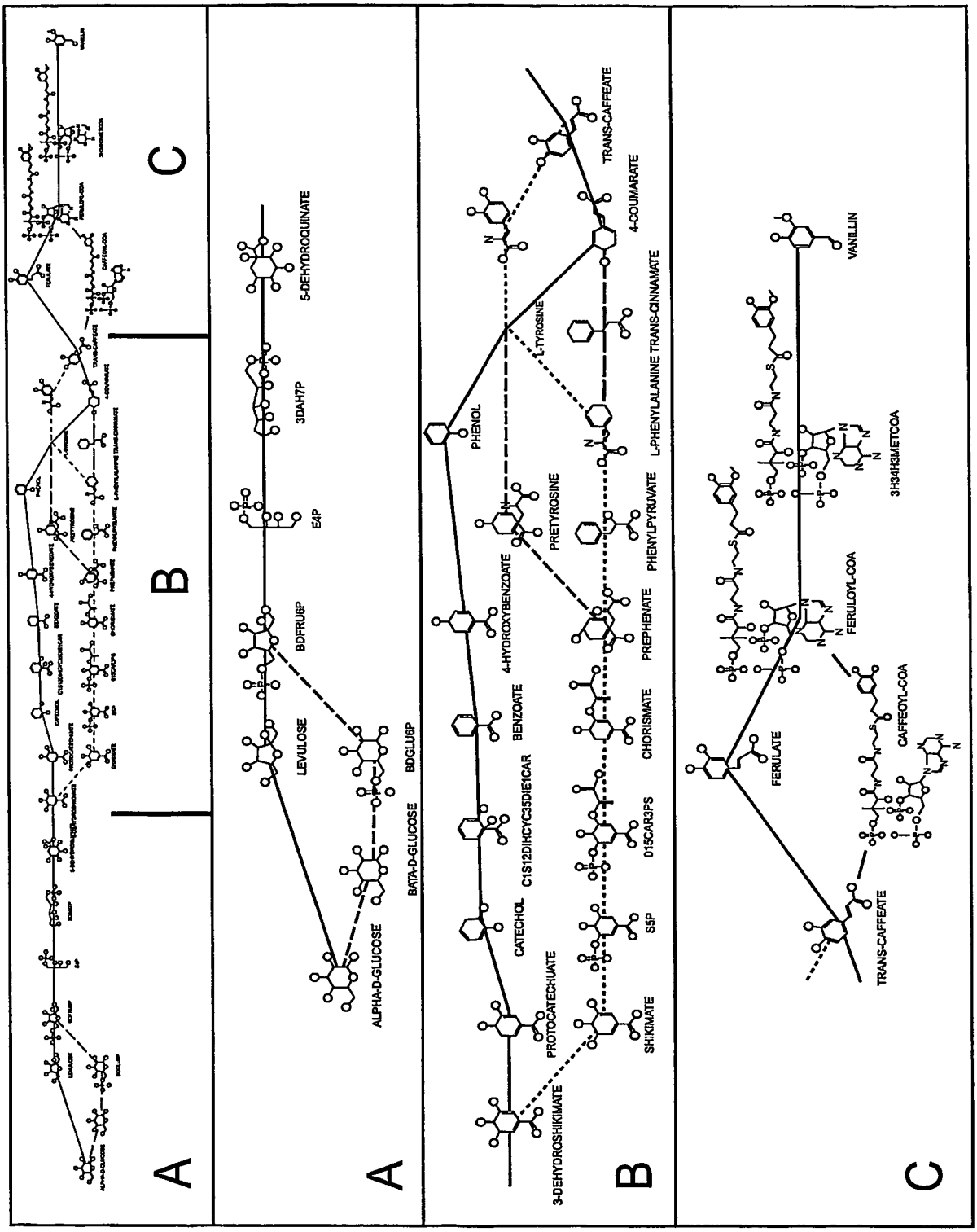

A
B
C
ALPHA-D-GLUCOSE
BATA-D-GLUCOSE
BDGLU6P
LEVULOSE
BDFRU6P
E4P
3DAH7P
5-DEHYDROQUINATE
3-DEHYDROSHIKIMATE
PROTOCATECHUATE
CATECHOL
C1S12DIHCYC3SDIE1CAR
BENZOATE
4-HYDROXYBENZOATE
PHENOL
SHIKIMATE
S5P
015CAR3PS
CHORISMATE
PREPHENATE
PHENYLPYRUVATE
PRETYROSINE
L-TYROSINE
L-PHENYLALANINE
TRANS-CINNAMATE
4-COUMARATE
TRANS-CAFFEATE
TRANS-CAFFEATE
FERULATE
CAFFEOYL-COA
FERULOYL-COA
3H34H3METCOA
VANILLIN

Fig. 14

LIGNIN
CONIFEROL
FERULALDEHYDE
FERULATE
TRANS-CAFFEATE
4-COUMARATE
4-HYDROXYBENZOATE
PROTOCATECHUATE
VANILLATE
VANILLIN

Fig. 15

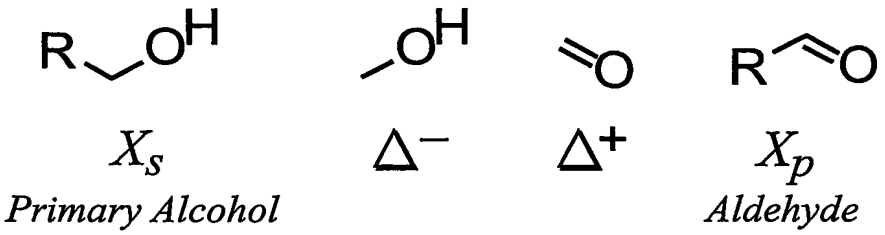


Fig. 16

Melatonin ⇔ *6 - Hydroxymelatonin*

Fatty Acid ⇔ **alphaHydroxy FattyAcid**

Alkane ⇔ **ROH**

Parthion ⇔ *Paraoxon*

Fig. 17

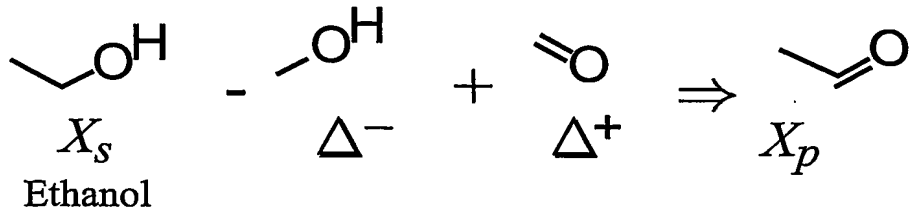


Fig. 18

```
input  : X_s, compound to metabolize
         Ū, list of rules
         n, iterations
output : Graphical visualization
         Products
Products ← φ
Γ_s ← molecular-graph(X_s)
for (Δ⁻, Δ⁺) ← Ū do
    Γ_p ← graph-replace(Γ_s, Δ⁻, Δ⁺)
    if Γ_p then
    X_p ← find-compound-by-graph(Γ_p)
    if X_p = φ then X_p ← make-novel-compound(Γ_p)
    pushnew(X_p, Products)
if n > 1 then
    for X in Products do
        append(metabolize(X, Ū, n − 1), Products)
```

Fig. 19

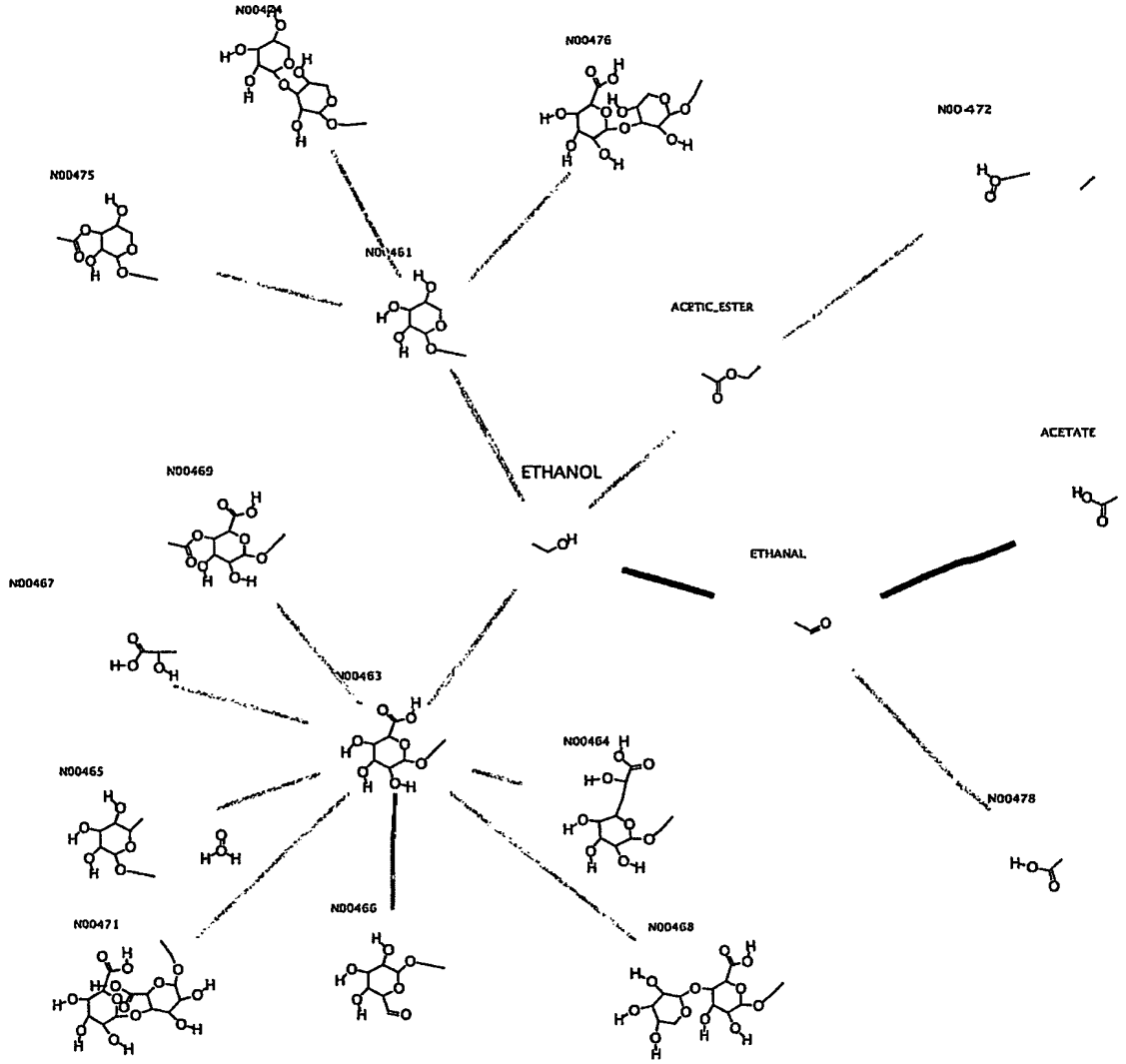
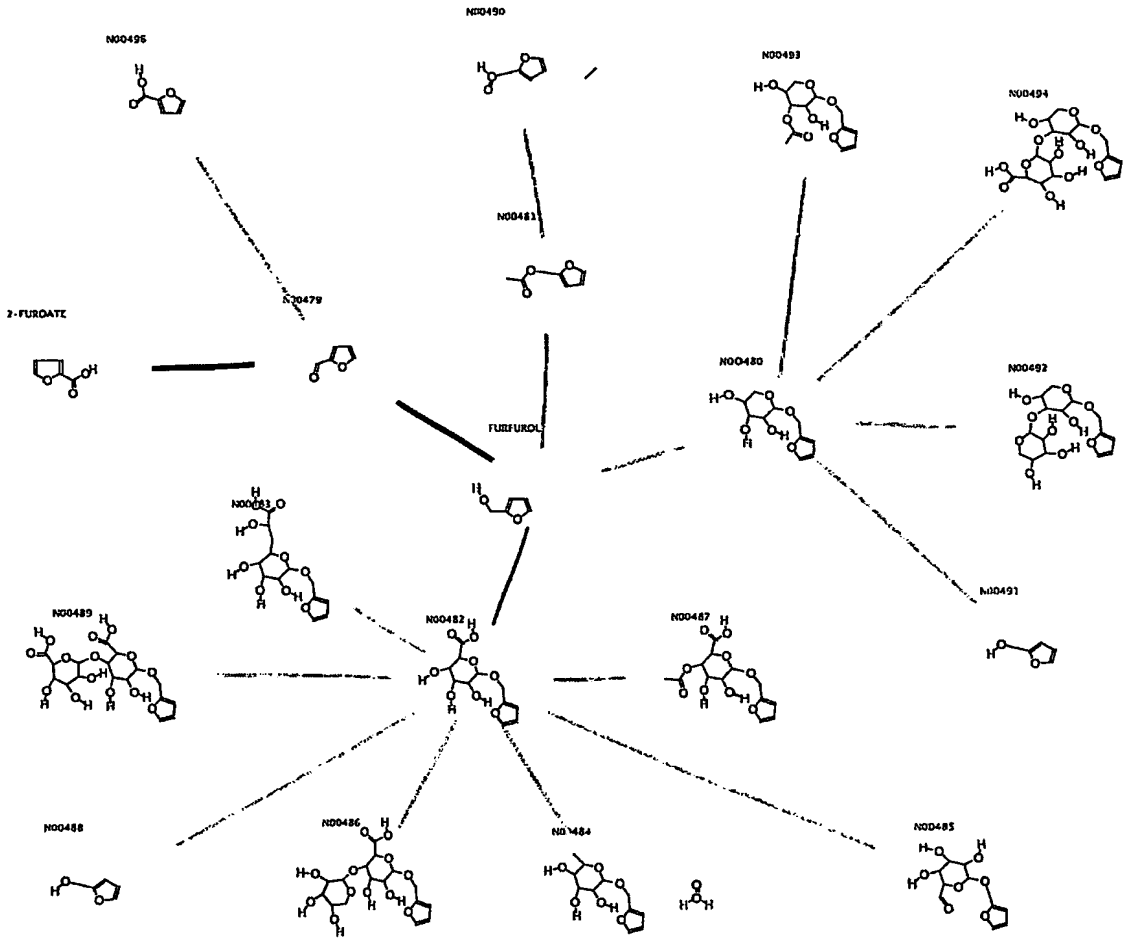

N00474
N00476
N00472
N00475
N00461
ACETIC_ESTER
ACETATE
ETHANOL
N00469
ETHANAL
N00467
N00463
N00464
N00465
N00478
N00466
N00471
N00468

Fig. 20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N00495
N00493
N00494
N00481
N00479
2-FUROATE
N00480
N00492
FURFUROL
N00491
N00489
N00482
N00487
N00488
N00486
N00484
N00485

Fig. 21